Massive, Distributed and Highly Accurate Computation of Particle Trajectories

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Summary

Scientists from the SciDAC Visualization and Analytics Center for Enabling Technology (VACET) have developed new capabilities for the analysis and visualization of very large vector field datasets with the aim of enabling rapid scientific knowledge discovery through state-of-the-art visualization methods. These new techniques leverage parallel computing platforms to significantly reduce the computational time required for computing particle trajectories in vector fields output from petascale simulations. Recent advances enable correct and reliable computation of particle trajectories in very large Adaptive Mesh Refinement (AMR) multi-grid datasets.

Figure 1. A path surface illustrates the flow of air around a car. The surface represents a dense sheet of massless particles, and the surface color coding provides insight into the lifetime of individual particles. The most notable features identified in this visualization are the vortices behind the rear-view mirror, where the particles are drawn into a vortex (close-up on the right). The path surface is constructed from several thousand integral curves.

Modern methods for the analysis and visualization of vector fields, which play a key role in many application domains like flow simulation, astrophysics and fusion, are built on empirically studying the behavior of massless particles advected with the vector field. These so-called *Lagrangian* methods offer unparalleled insight into vector field structures especially for time-dependent vector fields.

One simple, but quite effective, visualization approach for vector fields is the straightforward depiction of particle trajectories, as described by vector field integral curves and computed with the aid of numerical integration. Recently, VACET scientists have developed a novel approach of grouping trajectories of particles emanating from a common curve into so-called stream and path surfaces. The resulting visualizations – stream surfaces – are a significant improvement over visualizing individual curves due to the fact they offer the possibility for greatly improved visual understanding of complex 3D flow features.

Moreover, the recently introduced notion of *Finite-Time Lyapunov Exponents* (FTLE) has garnered much attention in both visualization and application science communities for its ability to visualize and analyze time-varying vector fields in terms of the convergence and divergence of neighboring particles. Having obtained such information, it is possible to accurately depict the fully dynamic nature of time varying vector fields. In contrast, earlier techniques are unable to easily capture time-varying structures. In addition, FTLE enables the representation of the structural dynamics in terms of scalar fields, opening up vector field structural analysis to a host of ex-

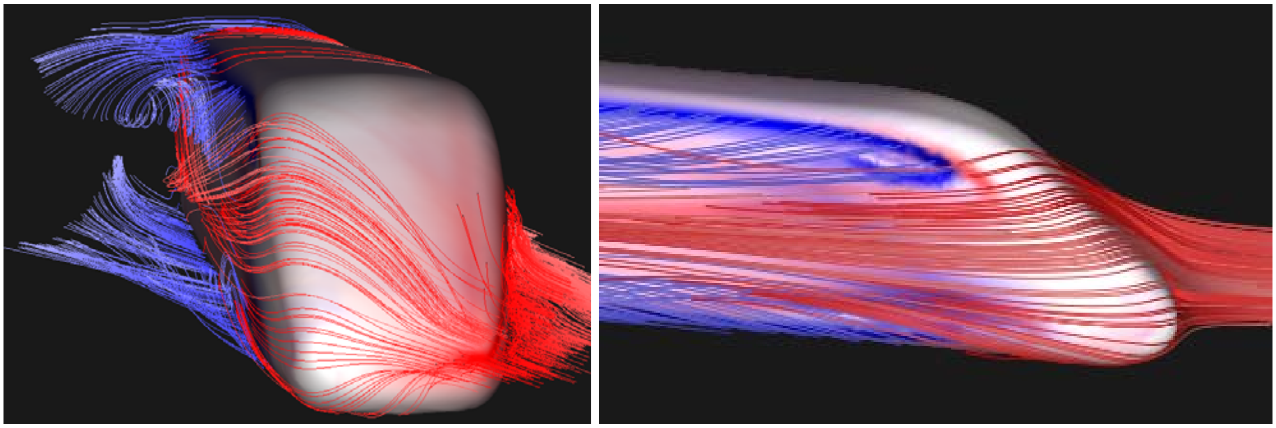

Figure 2. The Lagrangian visualization of the flow of air around the nose of a train reveals where sheets of air detach and reattach on the side of the train (blue corresponds to detachment, and red indicates re-attachment). This kind of analysis reveals indirect traces of large vortices forming close to the side of the train, and their study is important to determine the stability of the train at high speeds. Visualizing particle trajectories near the detachment and re-attachment zones (red and blue curves) using integral curves allows detailed insight into the flow structures.

isting methods in this context. VACET scientists have delivered visualization tools that enable fast computation and interactive visualization of vector fields using these Lagrangian techniques in its production-quality, parallel capable visual data analysis software infrastructure, VisIt.

Unfortunately, Lagrangian techniques require computing a huge number of particle traces that densely cover the domain of interest. Even for medium-sized datasets, it is not uncommon that application of Lagrangian visualization techniques requires computing millions of trace particles. In the past, VACET researchers have successfully worked to reduce the number of required particles, but the computational effort required to apply Lagrangian methods to very large, petascale datasets is still significant. This problem will be addressed by the development of novel parallelization techniques that will allow integral curve computation to scale to large supercomputers. These new capabilities, together with the Lagrangian visualization techniques that are build on them, will be implemented in production-quality, parallel-capable visual data exploration software that runs on virtually all modern platforms, ranging from desktop-class machines to DOE's petascale computer systems.

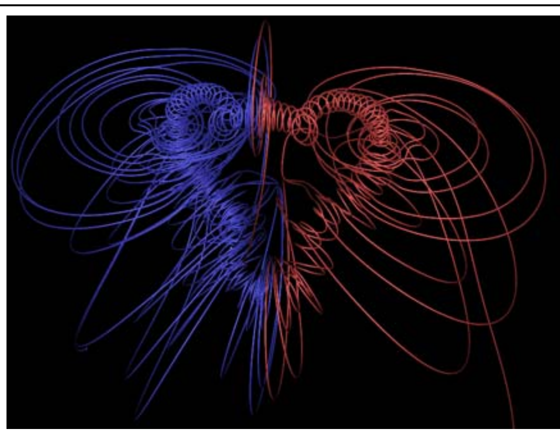

Figure 3. The figure depicts streamlines from an adaptive mesh refinement (AMR) computation of two incompressible vortex rings merging. In this time step, the vortex ring cores have already merged producing a complex flow field.

This represent a major new capability for domain scientists concerned with vector field analysis, as it will enable broad use of modern visualization methods and allow the treatment of petascale datasets when run on large parallel computing platforms.

Recent Publications

C. Garth, A. Wiebel, X. Tricoche, K. I. Joy, G. Scheuermann, *Lagrangian Visualization of Flow-Embedded Surface Structures*, in Computer Graphics Forum, Volume 27, Number 3, pp 1007--1014, 2008

C. Garth, H. Krishnan, X. Tricoche, T. Bobach, K. I. Joy, *Generation of Accurate Integral Surfaces in Time-Dependent Vector Fields*, in Proc. IEEE Visualization, 2008

Awards

People's Choice Award – SciDAC 2008.

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